

[Fe(OMe)₂(proline)]₁₂[ClO₄]₁₂ Structure: A7BCD15EF12_hP444_177_7n_n_jl_15n_n_12n-001

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<https://afLOW.org/p/TXX6>

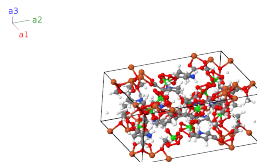
https://afLOW.org/p/A7BCD15EF12_hP444_177_7n_n_jl_15n_n_12n-001

Prototype	C ₇ ClFeH ₁₅ NO ₈
AFLOW prototype label	A7BCD15EF12_hP444_177_7n_n_jl_15n_n_12n-001
CCDC	222686
Pearson symbol	hP444
Space group number	177
Space group symbol	P622
AFLOW prototype command	afLOW --proto=A7BCD15EF12_hP444_177_7n_n_jl_15n_n_12n-001 --params=a, c/a, x ₁ , x ₂ , x ₃ , y ₃ , z ₃ , x ₄ , y ₄ , z ₄ , x ₅ , y ₅ , z ₅ , x ₆ , y ₆ , z ₆ , x ₇ , y ₇ , z ₇ , x ₈ , y ₈ , z ₈ , x ₉ , y ₉ , z ₉ , x ₁₀ , y ₁₀ , z ₁₀ , x ₁₁ , y ₁₁ , z ₁₁ , x ₁₂ , y ₁₂ , z ₁₂ , x ₁₃ , y ₁₃ , z ₁₃ , x ₁₄ , y ₁₄ , z ₁₄ , x ₁₅ , y ₁₅ , z ₁₅ , x ₁₆ , y ₁₆ , z ₁₆ , x ₁₇ , y ₁₇ , z ₁₇ , x ₁₈ , y ₁₈ , z ₁₈ , x ₁₉ , y ₁₉ , z ₁₉ , x ₂₀ , y ₂₀ , z ₂₀ , x ₂₁ , y ₂₁ , z ₂₁ , x ₂₂ , y ₂₂ , z ₂₂ , x ₂₃ , y ₂₃ , z ₂₃ , x ₂₄ , y ₂₄ , z ₂₄ , x ₂₅ , y ₂₅ , z ₂₅ , x ₂₆ , y ₂₆ , z ₂₆ , x ₂₇ , y ₂₇ , z ₂₇ , x ₂₈ , y ₂₈ , z ₂₈ , x ₂₉ , y ₂₉ , z ₂₉ , x ₃₀ , y ₃₀ , z ₃₀ , x ₃₁ , y ₃₁ , z ₃₁ , x ₃₂ , y ₃₂ , z ₃₂ , x ₃₃ , y ₃₃ , z ₃₃ , x ₃₄ , y ₃₄ , z ₃₄ , x ₃₅ , y ₃₅ , z ₃₅ , x ₃₆ , y ₃₆ , z ₃₆ , x ₃₇ , y ₃₇ , z ₃₇ , x ₃₈ , y ₃₈ , z ₃₈

- The oxygen sites labeled O-V through O-XII are only half filled.

Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B₁ =	$x_1 \mathbf{a}_1$	=	$\frac{1}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}}$	(6j)	Fe I
B₂ =	$x_1 \mathbf{a}_2$	=	$\frac{1}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}}$	(6j)	Fe I
B₃ =	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	=	$-ax_1 \hat{\mathbf{x}}$	(6j)	Fe I
B₄ =	$-x_1 \mathbf{a}_1$	=	$-\frac{1}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}}$	(6j)	Fe I
B₅ =	$-x_1 \mathbf{a}_2$	=	$-\frac{1}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}}$	(6j)	Fe I
B₆ =	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	=	$ax_1 \hat{\mathbf{x}}$	(6j)	Fe I
B₇ =	$x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	=	$-\sqrt{3}ax_2 \hat{\mathbf{y}}$	(6l)	Fe II
B₈ =	$x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2$	=	$\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}}$	(6l)	Fe II

$$\begin{aligned}
\mathbf{B}_{422} &= -y_{37} \mathbf{a}_1 + (x_{37} - y_{37}) \mathbf{a}_2 + z_{37} \mathbf{a}_3 = \frac{1}{2}a(x_{37} - 2y_{37}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{37} \hat{\mathbf{y}} + cz_{37} \hat{\mathbf{z}} & (12n) & \text{O XI} \\
\mathbf{B}_{423} &= -(x_{37} - y_{37}) \mathbf{a}_1 - x_{37} \mathbf{a}_2 + z_{37} \mathbf{a}_3 = -\frac{1}{2}a(2x_{37} - y_{37}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{37} \hat{\mathbf{y}} + cz_{37} \hat{\mathbf{z}} & (12n) & \text{O XI} \\
\mathbf{B}_{424} &= -x_{37} \mathbf{a}_1 - y_{37} \mathbf{a}_2 + z_{37} \mathbf{a}_3 = -\frac{1}{2}a(x_{37} + y_{37}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{37} - y_{37}) \hat{\mathbf{y}} + cz_{37} \hat{\mathbf{z}} & (12n) & \text{O XI} \\
\mathbf{B}_{425} &= y_{37} \mathbf{a}_1 - (x_{37} - y_{37}) \mathbf{a}_2 + z_{37} \mathbf{a}_3 = \frac{1}{2}a(-x_{37} + 2y_{37}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{37} \hat{\mathbf{y}} + cz_{37} \hat{\mathbf{z}} & (12n) & \text{O XI} \\
\mathbf{B}_{426} &= (x_{37} - y_{37}) \mathbf{a}_1 + x_{37} \mathbf{a}_2 + z_{37} \mathbf{a}_3 = \frac{1}{2}a(2x_{37} - y_{37}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{37} \hat{\mathbf{y}} + cz_{37} \hat{\mathbf{z}} & (12n) & \text{O XI} \\
\mathbf{B}_{427} &= y_{37} \mathbf{a}_1 + x_{37} \mathbf{a}_2 - z_{37} \mathbf{a}_3 = \frac{1}{2}a(x_{37} + y_{37}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{37} - y_{37}) \hat{\mathbf{y}} - cz_{37} \hat{\mathbf{z}} & (12n) & \text{O XI} \\
\mathbf{B}_{428} &= (x_{37} - y_{37}) \mathbf{a}_1 - y_{37} \mathbf{a}_2 - z_{37} \mathbf{a}_3 = \frac{1}{2}a(x_{37} - 2y_{37}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{37} \hat{\mathbf{y}} - cz_{37} \hat{\mathbf{z}} & (12n) & \text{O XI} \\
\mathbf{B}_{429} &= -x_{37} \mathbf{a}_1 - (x_{37} - y_{37}) \mathbf{a}_2 - z_{37} \mathbf{a}_3 = -\frac{1}{2}a(2x_{37} - y_{37}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{37} \hat{\mathbf{y}} - cz_{37} \hat{\mathbf{z}} & (12n) & \text{O XI} \\
\mathbf{B}_{430} &= -y_{37} \mathbf{a}_1 - x_{37} \mathbf{a}_2 - z_{37} \mathbf{a}_3 = -\frac{1}{2}a(x_{37} + y_{37}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{37} - y_{37}) \hat{\mathbf{y}} - cz_{37} \hat{\mathbf{z}} & (12n) & \text{O XI} \\
\mathbf{B}_{431} &= -(x_{37} - y_{37}) \mathbf{a}_1 + y_{37} \mathbf{a}_2 - z_{37} \mathbf{a}_3 = \frac{1}{2}a(-x_{37} + 2y_{37}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{37} \hat{\mathbf{y}} - cz_{37} \hat{\mathbf{z}} & (12n) & \text{O XI} \\
\mathbf{B}_{432} &= x_{37} \mathbf{a}_1 + (x_{37} - y_{37}) \mathbf{a}_2 - z_{37} \mathbf{a}_3 = \frac{1}{2}a(2x_{37} - y_{37}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{37} \hat{\mathbf{y}} - cz_{37} \hat{\mathbf{z}} & (12n) & \text{O XI} \\
\mathbf{B}_{433} &= x_{38} \mathbf{a}_1 + y_{38} \mathbf{a}_2 + z_{38} \mathbf{a}_3 = \frac{1}{2}a(x_{38} + y_{38}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{38} - y_{38}) \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII} \\
\mathbf{B}_{434} &= -y_{38} \mathbf{a}_1 + (x_{38} - y_{38}) \mathbf{a}_2 + z_{38} \mathbf{a}_3 = \frac{1}{2}a(x_{38} - 2y_{38}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{38} \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII} \\
\mathbf{B}_{435} &= -(x_{38} - y_{38}) \mathbf{a}_1 - x_{38} \mathbf{a}_2 + z_{38} \mathbf{a}_3 = -\frac{1}{2}a(2x_{38} - y_{38}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{38} \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII} \\
\mathbf{B}_{436} &= -x_{38} \mathbf{a}_1 - y_{38} \mathbf{a}_2 + z_{38} \mathbf{a}_3 = -\frac{1}{2}a(x_{38} + y_{38}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{38} - y_{38}) \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII} \\
\mathbf{B}_{437} &= y_{38} \mathbf{a}_1 - (x_{38} - y_{38}) \mathbf{a}_2 + z_{38} \mathbf{a}_3 = \frac{1}{2}a(-x_{38} + 2y_{38}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{38} \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII} \\
\mathbf{B}_{438} &= (x_{38} - y_{38}) \mathbf{a}_1 + x_{38} \mathbf{a}_2 + z_{38} \mathbf{a}_3 = \frac{1}{2}a(2x_{38} - y_{38}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{38} \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII} \\
\mathbf{B}_{439} &= y_{38} \mathbf{a}_1 + x_{38} \mathbf{a}_2 - z_{38} \mathbf{a}_3 = \frac{1}{2}a(x_{38} + y_{38}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{38} - y_{38}) \hat{\mathbf{y}} - cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII} \\
\mathbf{B}_{440} &= (x_{38} - y_{38}) \mathbf{a}_1 - y_{38} \mathbf{a}_2 - z_{38} \mathbf{a}_3 = \frac{1}{2}a(x_{38} - 2y_{38}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{38} \hat{\mathbf{y}} - cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII} \\
\mathbf{B}_{441} &= -x_{38} \mathbf{a}_1 - (x_{38} - y_{38}) \mathbf{a}_2 - z_{38} \mathbf{a}_3 = -\frac{1}{2}a(2x_{38} - y_{38}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{38} \hat{\mathbf{y}} - cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII} \\
\mathbf{B}_{442} &= -y_{38} \mathbf{a}_1 - x_{38} \mathbf{a}_2 - z_{38} \mathbf{a}_3 = -\frac{1}{2}a(x_{38} + y_{38}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{38} - y_{38}) \hat{\mathbf{y}} - cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII} \\
\mathbf{B}_{443} &= -(x_{38} - y_{38}) \mathbf{a}_1 + y_{38} \mathbf{a}_2 - z_{38} \mathbf{a}_3 = \frac{1}{2}a(-x_{38} + 2y_{38}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{38} \hat{\mathbf{y}} - cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII} \\
\mathbf{B}_{444} &= x_{38} \mathbf{a}_1 + (x_{38} - y_{38}) \mathbf{a}_2 - z_{38} \mathbf{a}_3 = \frac{1}{2}a(2x_{38} - y_{38}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{38} \hat{\mathbf{y}} - cz_{38} \hat{\mathbf{z}} & (12n) & \text{O XII}
\end{aligned}$$

References

- [1] A.-A. H. Abu-Nawwas, J. Cano, P. Christian, T. Mallah, G. Rajaraman, S. J. Teat, R. E. P. Winpenny, and Y. Yukawa, *An Fe(III) wheel with a zwitterionic ligand: the structure and magnetic properties of [Fe(OMe)₂(proline)]₁₂[ClO₄]₁₂*, Chem. Comm. pp. 314–315 (2004), doi:10.1039/B312947K.

Found in

- [1] F. Hoffmann, *The Fascination of Crystals and Symmetry* (2015). 230 – The Space Group List Project.

- C
- Cl
- Fe
- H
- N
- O

